

Introduction to GACRC Teaching Cluster PHYS4601/6601

Georgia Advanced Computing Resource Center (GACRC)

Enterprise Information Technology Services(EITS)

The University of Georgia



Outline

- GACRC
- Overview
- Working Environment
 - Two Nodes and Three Folders
 - Computational Partitions
 - Software
- Submit a Computational Batch Job
- GACRC Wiki and Support



GACRC

- A high-performance-computing (HPC) center at the UGA
- Provide to the UGA research and education community an advanced computing environment:
 - HPC computing and networking infrastructure located at the Boyd Data Center
 - Comprehensive collection of scientific, engineering and business applications
 - Consulting and training services

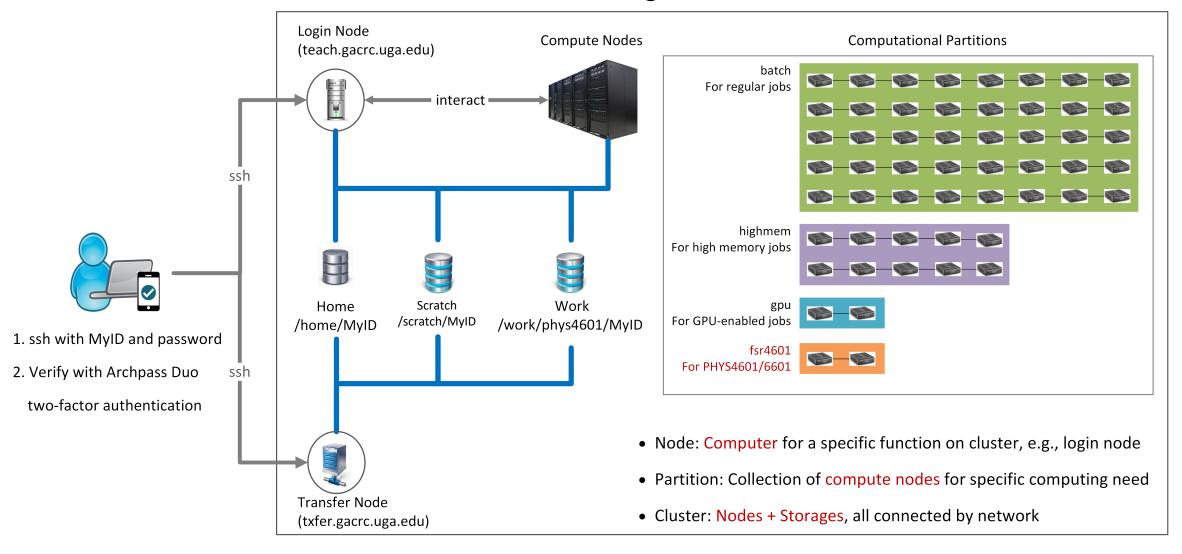
Wiki: http://wiki.gacrc.uga.edu

Support: https://wiki.gacrc.uga.edu/wiki/Getting_Help

Web Site: http://gacrc.uga.edu

Kaltura Channel: https://kaltura.uga.edu/channel/GACRC/176125031

Teaching Cluster



Note: You need to connect to the UGA VPN at first when accessing from outside of the UGA main campus.



Working Environment

https://wiki.gacrc.uga.edu/wiki/Systems#Teaching_cluster

- Two nodes, your "username" is your MyID for both of them:
 - 1. For batch job workflow, the host to log into is teach.gacrc.uga.edu
 - 2. For file transfers, the host to log into is txfer.gacrc.uga.edu
- > Three folders:
 - 1. /home/MyID : working space for running computational jobs
 - 2. /work/phys4601/MyID: data storing space for individual user in a class
 - 3. /work/phys4601/instructor_data: data shared with class by the instructors
- Partitions for PHYS4601/6601 class: fsr4601



Working Environment (cont.)

- Software
 - 1. Software names are long and have a Easybuild toolchain name associated to it
 - 2. Complete module name: Name/Version-toolchain, e.g., Python/3.10.4-GCCcore-11.3.0
 - Software names are case-sensitive!
 - module spider pattern: Search modules using a name pattern (case-insensitive)
 - > module load/unload moduleName: Load/remove a module
 - module avail: List all available modules on the cluster
 - module list:List modules currently loaded
 - > module purge: Remove all modules from working environment



Submit a Computational Batch Job

- Log on to Login node using MyID and password, and two-factor authentication with Archpass Duo: ssh MyID@teach.gacrc.uga.edu
- 2. Change directory to your scratch space: cd /scratch/MyID
- 3. Create a working subdirectory for a job: mkdir workDir
- 4. Change directory to workDir : cd workDir
- 5. Transfer data from local computer to workDir : use scp or WinSCP to connect Transfer node
 Transfer data on cluster to workDir : log on to Transfer node and then use cp or mv
- 6. Compile Fortran code *mult.f* into a binary code
- 7. Make a job submission script in workDir: nano sub.sh
- 8. Submit a job from workDir: sbatch sub.sh
- 9. Check job status : squeue --me or Cancel a job : scancel JobID



Step1: Log on to Login node

https://wiki.gacrc.uga.edu/wiki/Connecting#Connecting to the teaching cluster

- Teaching cluster access requires verification using two-factor authentication with
 Archpass Duo. If you are not enrolled in Archpass Duo, please refer to
 https://eits.uga.edu/access_and_security/infosec/tools/archpass_duo/ on how to enroll
- 2. If you are connecting from off-campus, please first connect to the UGA VPN and then connect to teach.gacrc.uga.edu. Information on how to use the VPN is available at https://eits.uga.edu/access_and_security/infosec/tools/vpn/



Step1: Log on to Login node - Mac/Linux using ssh

- 1. Open Terminal utility
- 2. Type command line: ssh MyID@teach.gacrc.uga.edu
- 3. You will be prompted for your UGA MyID password
- 4. You will verify your login using Archpass Duo authentication

ssh zhuofei@teach.gacrc.uga.edu 🖊 1. use ssh to open connection

UGA DUO authentication is required for SSH/SCP access to GACRC systems. For additional help with UGA DUO authentication or to report an issue please visit: https://eits.uga.edu/access_and_security...

Password:

2. Enter your MyID password
When you enter password, no stars or dots will show as you are typing. Please type password carefully!

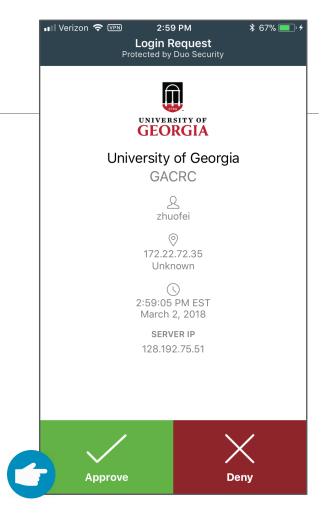
Duo two-factor login for zhuofei

Enter a passcode or select one of the following options:

- 1. Duo Push to XXX-XXX-5758
- 2. Phone call to XXX-XXX-5758
- 3. Phone call to XXX-XXX-1925
- 4 5. SMS passcodes to XXX-XXX-5758 (next code starts with: 1)

Success. Logging you in...

Last login: Mon Aug 3 11:11:58 2020 from 172.18.114.119



5. Verify login using Duo



Step1 (Cont.) - Windows using PuTTY

- Download and install PuTTY: https://www.putty.org/
- 2. Detailed downloading and installation instructions:

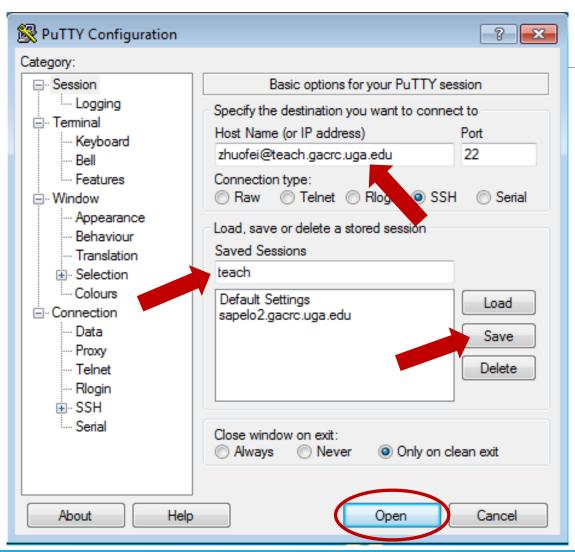
https://wiki.gacrc.uga.edu/wiki/How_to_Install_and_Configure_PuTTY

3. Detailed configuring and usage instructions:

https://wiki.gacrc.uga.edu/wiki/How_to_Install_and_Configure_PuTTY#Configuring_PuTTY

Step1 (Cont.) - Windows using PuTTY





The first time you connect to login node, PuTTY will give you this security alert window. Please click "Yes"



Step1 (Cont.) - Windows using PuTTY



Next you will enter your UGA MyID password and initiate DUO authentication procedure:

```
zhuofei@teach-sub1:~
                                                                     - - X
  Using username "zhuofei".
  Keyboard-interactive authentication prompts from server:
 Password:
                        ← UGA MyID password
 Duo two-factor login for zhuofei
 Enter a passcode or select one of the following options:

    Duo Push to XXX-XXX-5758

  2. Phone call to XXX-XXX-5758
  3. Phone call to XXX-XXX-1925
  4. Phone call to XXX-XXX-3535
  5. SMS passcodes to XXX-XXX-5758
 Passcode or option (1-5): 1  Select DUO option
  End of keyboard-interactive prompts from server
Success. Logging you in...
Last login: Thu Jan 7 10:20:01 2021 from 128.192.240.123
zhuofei@teach-sub1 ~$ _____ Logged on!
```



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Step2 - 4: cd to /scratch dir, make and cd into workDir

Step5: Transfer data from local computer to workDir - Mac/Linux

https://wiki.gacrc.uga.edu/wiki/Transferring_Files#Using_scp_2

- 1. Connect to Transfer node (txfer.gacrc.uga.edu) in Terminal from your local computer
- 2. Use scp command: scp (-r) [Source] [Target]
- 3. Enter your MyID password, then select Duo option to verify connection

E.g. 1: use scp on local computer, from Local → workDir on cluster

```
scp ./file zhuofei@txfer.gacrc.uga.edu:/home/zhuofei/workDir
scp -r ./folder/ zhuofei@txfer.gacrc.uga.edu:/home/zhuofei/workDir
```

E.g. 2: use scp on local computer, from workDir on cluster → Local

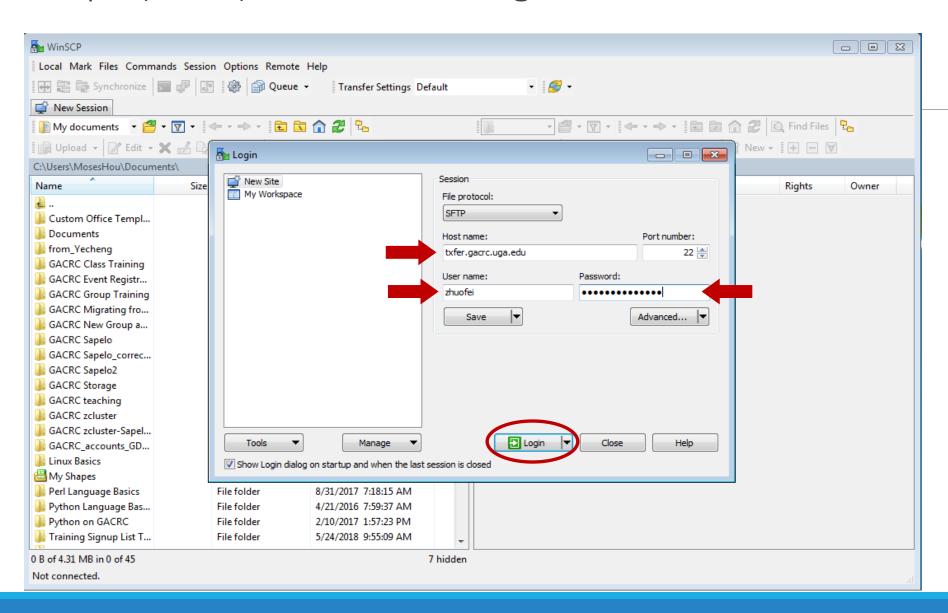
```
scp zhuofei@txfer.gacrc.uga.edu:/home/zhuofei/workDir/file .
scp -r zhuofei@txfer.gacrc.uga.edu:/home/zhuofei/workDir/folder/ .
```



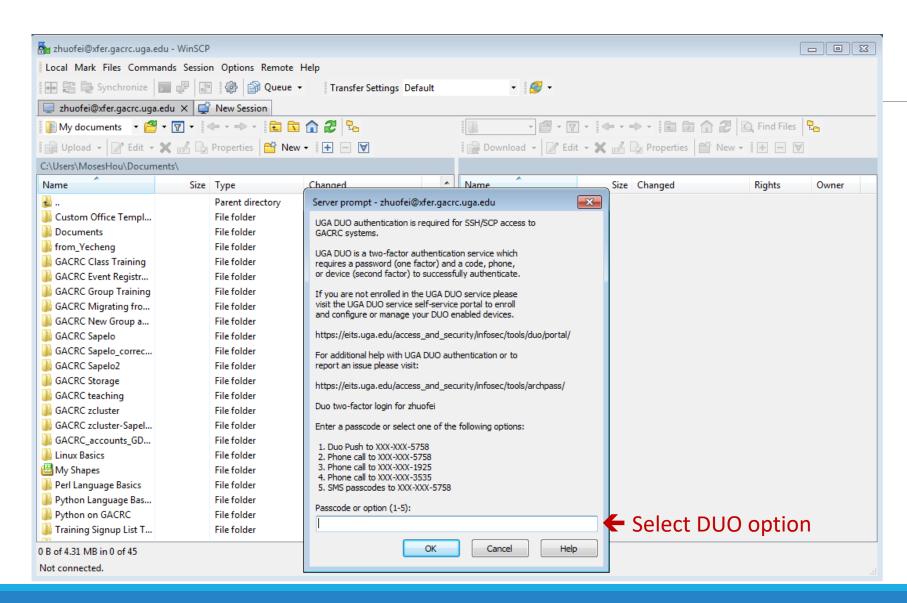
https://wiki.gacrc.uga.edu/wiki/Transferring_Files#Using_WinSCP_2

- 1. You need to connect to cluster's <u>Transfer node</u> (txfer.gacrc.uga.edu)
- 2. Use WinSCP on local computer
 - WinSCP can be downloaded from https://winscp.net/eng/index.php
 - Default installation procedure is simple
- 3. Alternative FileZilla https://wiki.gacrc.uga.edu/wiki/Transferring-Files#Using-FileZilla-2

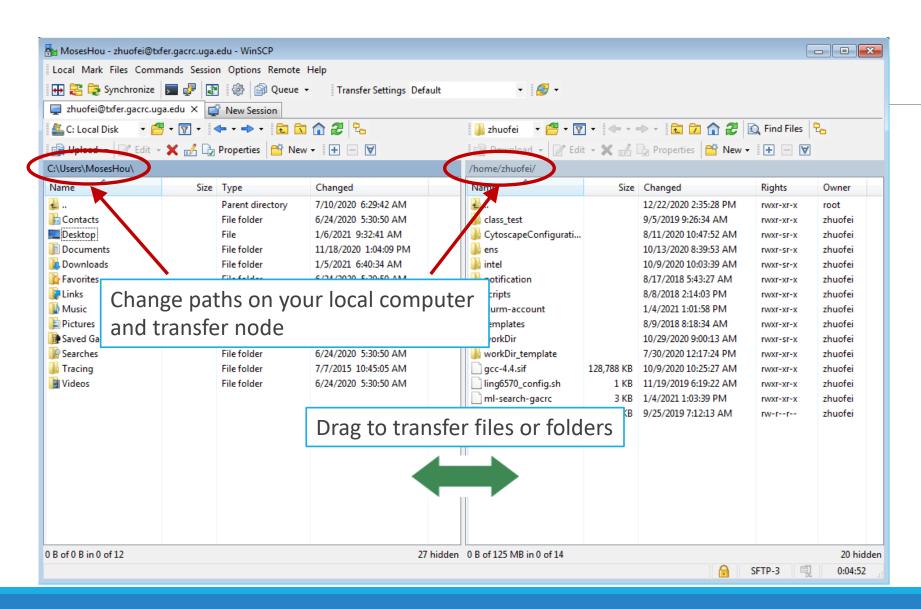














Step5 (Cont.): Transfer data on cluster to workDir

- Log on to Transfer node (txfer.gacrc.uga.edu)
 - ✓ Mac/Linux: ssh MyID@txfer.gacrc.uga.edu (page 9-10)
 - ✓ Windows: use PuTTY to log in MyID@txfer.gacrc.uga.edu (page 11-13)
- Directories you can access on transfer node:
 - /home/MyID (Landing home)
 - 2. /work/phys4601/MyID
 - 3. /work/phys4601/instructor_data
- Transfer data between two folders on cluster using cp or mv, e.g.:

mv /work/phys4601/MyID/datafile /home/MyID/workDir

Step6: Compile Fortran code *mult.f* into a binary



```
zhuofei@teach-sub1 workDir$ interact
zhuofei@tcn26 workDir$ cp /usr/local/gacrc/training/phys4601/mult.f . 	Copy source code to your working dir
zhuofei@tcn26 workDir$ cat mult.f
   Program mult
C Multiplies two integer numbers
   implicit none
   integer i,j,iprod
   i=3
   i=4
   open(1, file='output.txt')
   iprod=i*j
   write(1,10)i,j,iprod
10 format('The product of ', I2, ' and ', I2, ' is ', I3)
   close(1)
   end
zhuofei@tcn26 workDir$ module load GCC/11.3.0
zhuofei@tcn26 workDir$ gfortran mult.f -o mult.x
zhuofei@tcn26 workDir$ ls
mult.f mult.x
zhuofei@tcn26 workDir$ exit
```

- ← Start an interactive session
- ← Show contents of source code

- ← Load GCC compiler module
- ← Compile source code into a binary
- Elinary is generated in your working dir
- Exit from interactive session

Step7: Make a job submission script sub.sh using nano



```
zhuofei@teach-sub1 workDir$ cp /usr/local/gacrc/training/phys4601/sub.sh .
                                                                               Copy sub.sh to working dir
zhuofei@teach-sub1 workDir$ cat sub.sh
                                                                               ← Show contents of sub.sh
#!/bin/bash
                                         # Job name
#SBATCH --job-name=test
#SBATCH --partition=fsr4601
                                         # Submit job to fsr4601 partition
#SBATCH --ntasks=1
                                         # Single task job
                                         # Number of cores per task
#SBATCH --cpus-per-task=1
#SBATCH --mem=2gb
                                         # Total memory for job
#SBATCH --time=00:01:00
                                         # Time limit hrs:min:sec; fsr4601 TIMELIMIT 1 min
#SBATCH --output=log.%j
                                         # Standard output and error log
#SBATCH --mail-user=MyID@uga.edu
                                         # Where to send mail
                                         # Mail events (BEGIN, END, FAIL, ALL)
#SBATCH --mail-type=ALL
cd $SLURM_SUBMIT_DIR
module load GCC/11.3.0
time ./mult.x
                                         # run the binary code you compiled in step 5 in this job
zhuofei@teach-sub1 workDir$ nano sub.sh
                                              ← Use nano modify sub.sh, e.g., email address
```



Step8: Submit a job from workDir using sbatch

https://wiki.gacrc.uga.edu/wiki/Running Jobs on the teaching cluster#How to submit a job to the batch queue

\$ sbatch sub.sh
Submitted batch job 5230

Tips: sub.sh is a job submission script for

- 1. specifying computing resources
- 2. loading compiler module using module load
- 3. running any Linux commands you want to run
- 4. running your binary code



Step9: Check job status using squeue

https://wiki.gacrc.uga.edu/wiki/Monitoring Jobs on the teaching cluster

```
zhuofei@teach-sub1 workDir$ squeue --me
JOBID PARTITION
                     NAME
                               USER
                                      ST
                                                TIME
                                                      NODES NODELIST (REASON)
 5230
        fsr4601
                            zhuofei
                                                0:01
                                                           1 \text{ rb} 1 - 3
                     test
zhuofei@teach-sub1 workDir$ squeue --me -1
Mon Jan 09 26:03:14 2024
JOBID
      PARTITION
                                                     TIME TIME LIMI
                     NAME
                               USER
                                        STATE
                                                                       NODES NODELIST (REASON)
 5230
        fsr4601
                            zhuofei
                                                     0:05
                                                                1:00
                                                                           1 rb1-3
                     test
                                      RUNNING
```

Job State: R for Running; PD for PenDing; F for Failed

TIME: the elapsed time used by the job, not remaining time, not CPU time



Step9 (Cont.): Cancel job using scancel

https://wiki.gacrc.uga.edu/wiki/Running Jobs on the teaching cluster#How to delete a running or pending job

```
zhuofei@teach-sub1 workDir$ scancel 5230
zhuofei@teach-sub1 workDir$ squeue --me

JOBID PARTITION NAME USER ST TIME NODES NODELIST(REASON)
```



Step9 (Cont.): Check job details using sacct-gacrc -X and seff

https://wiki.gacrc.uga.edu/wiki/Monitoring Jobs on the teaching cluster

\$ sacct-gacrc -X

JobID	JobName	User	Partition	NNode NCPUS	ReqMem	CPUTime	Elapsed	Timelimit	State	ExitCode	NodeList	
5230	 test zl	 nuofei	 fsr4601	 1 1	 2G	 00:00:01	 .00:00:01	00.01.00	COMPLETED	0.0	 rb1-3	

\$ seff 5230 # Check computing resources used by a COMPLETED job

Cluster: gacrc-teach

User/Group: zhuofei/gacrc-instruction

State: COMPLETED (exit code 0)

Cores: 1

CPU Utilized: 00:00:00

CPU Efficiency: 0.00% of 00:00:01 core-walltime

Job Wall-clock time: 00:00:01

Memory Utilized: 0.00 MB (estimated maximum)

Memory Efficiency: 0.00% of 2.00 GB (2.00 GB/node)



Step9 (Cont.): Check node info using sinfo

https://wiki.gacrc.uga.edu/wiki/Monitoring Jobs on the teaching cluster

zhuofei@teach-sub1 workDir\$ sinfo									
PARTITION	AVAIL	TIMELIMIT	NODES	STATE	NODELIST				
allnodes	up	infinite	1	mix	rb1-11				
allnodes	up	infinite	12	idle	c4-23,rb1-[1-10,12]				
batch	up	7-00:00:00	8	idle	rb1-[3-10]				
gpu	up	7-00:00:00	1	idle	c4-23				
highmem	up	7-00:00:00	2	idle	rb1-[1-2]				
Interactive	up	7-00:00:00	1	mix	rb1-11				
interactive	up	7-00:00:00	1	idle	rb1-12				
fsr4601	up	1:00	8	idle	rb1-[3-10]				
fsr8602	up	10:00	8	idle	rb1-[3-10]				

idle = no cores in use; mix = some cores are still free; alloc = all cores are allocated



Obtain Job Details

https://wiki.gacrc.uga.edu/wiki/Running_Jobs_on_the_teaching_cluster#How_to_check_resource_utilization_of_a_running_or_finished_job

Option 1: seff for details of computing resource usage of a finished job

Option 2: sacct-gacrc for details of computing resource usage of a running or finished job

Option 3: Email notification from finished jobs (completed, canceled, or crashed), if using:

```
#SBATCH --mail-user=username@uga.edu
```

```
#SBATCH --mail-type=ALL
```



GACRC Wiki http://wiki.gacrc.uga.edu Kaltura Channel https://kaltura.uga.edu/channel/GACRC/176125031

Connecting: https://wiki.gacrc.uga.edu/wiki/Connecting#Connecting to the teaching cluster

Running Jobs: https://wiki.gacrc.uga.edu/wiki/Running_Jobs_on_the_teaching_cluster

Monitoring Jobs: https://wiki.gacrc.uga.edu/wiki/Monitoring_Jobs_on_the_teaching_cluster

Transfer File:

https://wiki.gacrc.uga.edu/wiki/Transferring_Files#The_File_Transfer_node_for_the_teaching_cluster_.

28txfer.gacrc.uga.edu.29

Sample Job Scripts:

https://wiki.gacrc.uga.edu/wiki/Sample_batch_job_submission_scripts_on_the_teaching_cluster

Linux Command: https://wiki.gacrc.uga.edu/wiki/Command_List



GACRC Support

https://wiki.gacrc.uga.edu/wiki/Getting_Help

Job Troubleshooting:

Please tell us details of your question or problem, including but not limited to:

- ✓ Your user name
- ✓ Your job ID
- ✓ Your working directory
- ✓ The partition name and command you used to submit the job

Software Installation:

- ✓ Specific name and version of the software
- ✓ Download website
- ✓ Supporting package information if have

Please note to make sure the correctness of datasets being used by your jobs!



Search the client portal



Zhuofei Hou

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My Recent My Approvals

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Search

Service Catalog / Academics, Learning & Research / GACRC Service Catalog

GACRC Service Catalog

Georgia Advanced Computing Resource Center (GACRC) service catalog.

If you would like to reach out to GACRC and do not have a UGA MyID, please send an email to gacrchelp@uga.edu, and we will respond promptly.

Categories (3)



Services For Users

General user support, request software installation or update, request training.

Services for PIs

For PIs only: Lab registration, user account creation/modification, class account requests, storage quota modifications.

For GACRC Staff

For GACRC's internal use only.

My Recent Requests

Class provision on the teaching cluster - phys8601dlandau

Class provision on the teaching cluster - bcmb8330 - rjwoods

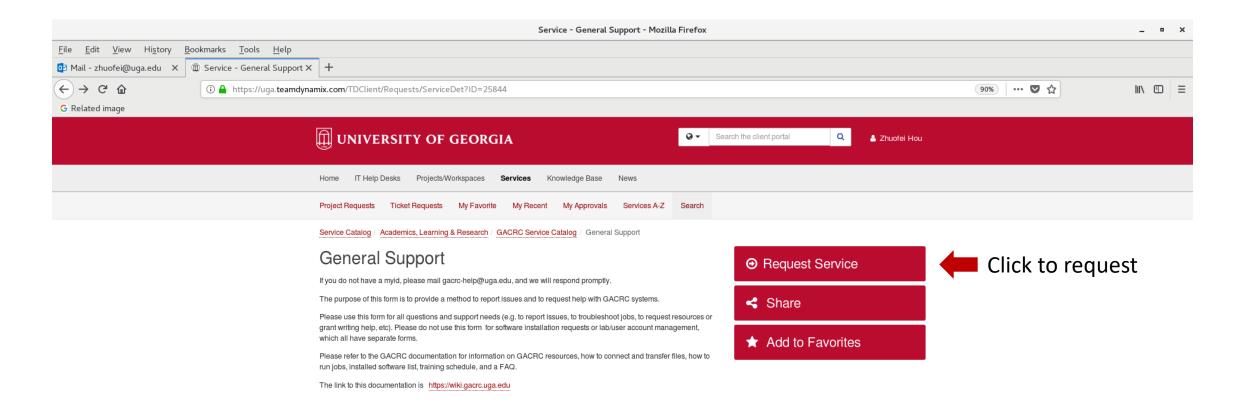
Class provision on the teaching cluster - binf8211 - szhao, lm43161

MATLAB License Request

Create cider lab group

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https://uga.teamdynamix.com/TDClient/Requests/ServiceCatalogSearch

Need Support? http://help.gacrc.uga.edu

